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Conformation and Proton Configuration of Pyrimidine Deoxynucleoside Oxidation Damage Products in Water

Christopher J. La Francois, Yun Hee Jang, Tahir Cagin, William A. Goddard, III and Lawrence C. Sowers

Supplementary table #1. The final structure of protonated HODCTP. The below listing of coordinates corresponds to the structure shown in Fig. 8A

HEADER	PROTEIN									
COMPND	supp_HODCMP_solv.01.pdb									
AUTHOR	GENERATED BY BABEL 1.3									
ATOM	1	N	UNK	1	4.772	5.124	8.578	1.00	0.00	
ATOM	2	C	UNK	1	3.927	5.974	9.247	1.00	0.00	
ATOM	3	N	UNK	1	4.340	7.229	9.522	1.00	0.00	
ATOM	4	C	UNK	1	5.557	7.607	9.214	1.00	0.00	
ATOM	5	C	UNK	1	6.533	6.669	8.760	1.00	0.00	
ATOM	6	C	UNK	1	6.079	5.464	8.403	1.00	0.00	
ATOM	7	O	UNK	1	2.804	5.588	9.541	1.00	0.00	
ATOM	8	N	UNK	1	5.904	8.891	9.374	1.00	0.00	
ATOM	9	C	UNK	1	4.161	3.954	7.901	1.00	0.00	
ATOM	10	C	UNK	1	3.052	4.375	6.917	1.00	0.00	
ATOM	11	C	UNK	1	3.409	3.676	5.611	1.00	0.00	
ATOM	12	C	UNK	1	4.905	3.406	5.745	1.00	0.00	
ATOM	13	O	UNK	1	5.127	3.290	7.150	1.00	0.00	
ATOM	14	O	UNK	1	2.685	2.468	5.529	1.00	0.00	
ATOM	15	C	UNK	1	5.776	4.478	5.131	1.00	0.00	
ATOM	16	O	UNK	1	5.366	5.718	5.628	1.00	0.00	
ATOM	17	O	UNK	1	7.650	6.755	5.948	1.00	0.00	
ATOM	18	O	UNK	1	6.325	7.220	3.873	1.00	0.00	
ATOM	19	O	UNK	1	5.536	8.129	6.107	1.00	0.00	
ATOM	20	P	UNK	1	6.276	7.054	5.372	1.00	0.00	
ATOM	21	H	UNK	1	5.157	9.555	9.418	1.00	0.00	
ATOM	22	H	UNK	1	6.716	9.193	8.878	1.00	0.00	
ATOM	23	O	UNK	1	7.805	7.085	8.522	1.00	0.00	
ATOM	24	H	UNK	1	6.710	4.739	7.940	1.00	0.00	
ATOM	25	H	UNK	1	3.804	3.284	8.666	1.00	0.00	
ATOM	26	H	UNK	1	3.069	5.445	6.778	1.00	0.00	
ATOM	27	H	UNK	1	2.073	4.084	7.268	1.00	0.00	
ATOM	28	H	UNK	1	3.188	4.294	4.750	1.00	0.00	
ATOM	29	H	UNK	1	5.171	2.451	5.307	1.00	0.00	
ATOM	30	H	UNK	1	2.897	2.035	4.708	1.00	0.00	
ATOM	31	H	UNK	1	5.667	4.441	4.052	1.00	0.00	
ATOM	32	H	UNK	1	6.814	4.286	5.373	1.00	0.00	
ATOM	33	H	UNK	1	7.894	7.078	7.547	1.00	0.00	
CONNECT	1	2	6	9						
CONNECT	2	1	3	7						
CONNECT	3	2	4							
CONNECT	4	3	5	8						
CONNECT	5	4	6	23						

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Conformation and Proton Configuration of Pyrimidine Deoxynucleoside Oxidation Damage Products in Water

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Supplementary table #2. The final structure of ionized OdCTP. The below listing of coordinates corresponds to the structure shown in Fig. 8B

HEADER	PROTEIN									
COMPND	supp OdCMP solv.01.pdb									
AUTHOR	GENERATED BY BABEL 1.3									
ATOM	1	N	UNK	1	4.546	5.802	9.265	1.00	0.00	
ATOM	2	C	UNK	1	4.394	5.501	10.576	1.00	0.00	
ATOM	3	N	UNK	1	4.835	6.391	11.505	1.00	0.00	
ATOM	4	C	UNK	1	5.403	7.512	11.143	1.00	0.00	
ATOM	5	C	UNK	1	5.647	7.889	9.744	1.00	0.00	
ATOM	6	C	UNK	1	5.191	6.981	8.870	1.00	0.00	
ATOM	7	O	UNK	1	3.857	4.453	10.934	1.00	0.00	
ATOM	8	N	UNK	1	5.811	8.373	12.066	1.00	0.00	
ATOM	9	C	UNK	1	4.046	4.911	8.236	1.00	0.00	
ATOM	10	C	UNK	1	3.104	5.582	7.235	1.00	0.00	
ATOM	11	C	UNK	1	3.952	5.817	5.987	1.00	0.00	
ATOM	12	C	UNK	1	5.060	4.762	6.115	1.00	0.00	
ATOM	13	O	UNK	1	5.134	4.427	7.487	1.00	0.00	
ATOM	14	O	UNK	1	3.181	5.689	4.830	1.00	0.00	
ATOM	15	C	UNK	1	6.450	5.240	5.725	1.00	0.00	
ATOM	16	O	UNK	1	6.488	5.809	4.444	1.00	0.00	
ATOM	17	O	UNK	1	6.990	3.596	3.362	1.00	0.00	
ATOM	18	O	UNK	1	4.780	4.730	2.949	1.00	0.00	
ATOM	19	O	UNK	1	6.893	5.740	2.020	1.00	0.00	
ATOM	20	P	UNK	1	6.279	4.891	3.099	1.00	0.00	
ATOM	21	H	UNK	1	5.584	8.233	13.026	1.00	0.00	
ATOM	22	H	UNK	1	6.139	9.265	11.763	1.00	0.00	
ATOM	23	O	UNK	1	6.246	9.000	9.497	1.00	0.00	
ATOM	24	H	UNK	1	5.311	7.129	7.821	1.00	0.00	
ATOM	25	H	UNK	1	3.583	4.087	8.742	1.00	0.00	
ATOM	26	H	UNK	1	2.671	6.494	7.625	1.00	0.00	
ATOM	27	H	UNK	1	2.300	4.901	6.988	1.00	0.00	
ATOM	28	H	UNK	1	4.392	6.808	6.002	1.00	0.00	
ATOM	29	H	UNK	1	4.779	3.880	5.551	1.00	0.00	
ATOM	30	H	UNK	1	3.753	5.381	4.111	1.00	0.00	
ATOM	31	H	UNK	1	7.156	4.423	5.802	1.00	0.00	
ATOM	32	H	UNK	1	6.758	6.013	6.417	1.00	0.00	
CONNECT	1	2	6	9						
CONNECT	2	1	3	7						
CONNECT	3	2	4							
CONNECT	4	3	5	8						
CONNECT	5	4	6	23						

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